Dislocation core field. I. Modeling in anisotropic linear elasticity theory

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Aside from the Volterra field, dislocations create a core field, which can be modeled in linear anisotropic elasticity theory with force and dislocation dipoles. We derive an expression of the elastic energy of a dislocation taking full account of its core field and show that no cross term exists between the Volterra and the core fields. We also obtain the contribution of the core field to the dislocation interaction energy with an external stress, thus showing that dislocation can interact with a pressure. The additional force that derives from this core field contribution is proportional to the gradient of the applied stress. Such a supplementary force on dislocations may be important in high stress gradient regions, such as close to a crack tip or in a dislocation pile-up.

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I. INTRODUCTION

Far from a dislocation, the elastic field is well described by the Volterra solution[1]: this predicts that the displacement and the stress are respectively varying proportionally to the logarithm and the inverse of the distance to the dislocation. But the elastic field may deviate from this ideal solution close to the dislocation. Such a deviation corresponds to the dislocation core field. It arises from anharmonicities in the crystal elastic behavior, especially in the high-strained region of the core, as well as from perturbations caused by the atomic nature of the core. It is, in part, responsible for the dislocation formation volume, which manifests itself experimentally[2] through an increase of the lattice parameter with the dislocation density. This leads to an interaction of the dislocation with an external pressure[3]. Although the core field decays more rapidly than the Volterra field, it can modify the elastic interaction of dislocations with other defects[4–6]. For instance, equilibrium distances in a dislocation pile-up are affected by this core field[7]. As a consequence, the stress concentration at the tip of the pile-up is enhanced. This can favor fracture initiation or yielding for an edge or mixed dislocation pile-up, or cross-slip for a screw pile-up[7]. The stress produced by this core field also tends to open the crack in front of the dislocation pile-up on the glide plane[8]. This explains the nucleation of a crack in a mixed mode I-II or I-III sometimes observed experimentally in the glide plane of the pile-up. Without the core field, only modes II and III would be possible. The core field can also alter dislocation properties such as their elastic energy[6,9] or their dissociation distance in fcc metals[4,5]. Finally, it contributes to the elastic interaction between dislocations and impurities, and thus may explain part of the solid solution hardening[10].

One can use atomistic simulations, either based on empirical potentials or on *ab initio* calculations, so as to take full account of the core field when studying dislocations. On the other hand, the core field can be modeled within linear elasticity theory, using an equilibrated distribution of line forces parallel to the dislocation and located close to its core[9,11–13]. A multipole expansion of the distribution leads then to an expression of the core field in term of a series. Usually, only the leading term of this series is considered. The core field is then equivalent to an elliptical line source expansion and is fully characterized by the first moments of the line force distribution. Comparison with atomistic simulations have shown that this approach correctly describes the dislocation core field[4,5,9,12,14].

Until now, only few studies[4,5,7,9] have included this core field in the calculation of the elastic energy of dislocations or of their interaction with an external stress field. Most of the time, dislocation elastic energies are obtained by considering only the Volterra elastic field. Such an approximated approach may lead to some errors. Notably, simulation boxes used within *ab initio* calculations are usually too small to neglect the core field. A recent study of the screw dislocation in iron[6] has shown, indeed, that it is necessary to include this core field in the computation of the elastic energy when deriving core energies from *ab initio* calculations. The purpose of this paper is to extend the modeling approach[11] of the core field within anisotropic linear elasticity so as to include its contribution in energy calculations. Previous studies, which have considered this core field contribution, either assumed that the elastic behavior is isotropic[4,5,7,9], or that the elastic constants obey a given symmetry[5,11] incompatible for instance with a $\langle 111 \rangle$ screw dislocation in a cubic crystal.

In this paper, we first review how the elastic field of a line defect, including the core field, is modeled within linear anisotropic elasticity theory. The approach of Hirth and Lothe[11] is generalized so as to describe the core field not only through a distribution of line forces but also a distribution of dislocations. The elastic energy of the line defect is then computed, thus showing the extra contribution arising from the core field. Finally, we determine the influence of the core field on the interaction of the line defect with an external stress.

II. ELASTIC FIELD OF A LINE DEFECT

We consider a static line defect, the line direction of which is denoted $\mathbf{e}_3$. Such a defect can be either a dislocation, a line force, or the combination of both. Eshelby *et al.*[15] have shown that the elastic displacement and the stress created at a point of coordinates $\mathbf{x}$ can be, respectively, written as

$$u_k(\mathbf{x}) = \frac{1}{2}\sum_{\alpha=1}^{6} A_k^\alpha f_\alpha[z_\alpha], \tag{1a}$$

$$\sigma_{ij}(\mathbf{x}) = \frac{1}{2}\sum_{\alpha=1}^{6} B_{ijk}^\alpha A_k^\alpha \frac{\partial f_\alpha[z_\alpha]}{\partial z_\alpha}, \tag{1b}$$

where the variable z_α is related to Cartesian coordinates by $z_\alpha = x_1 + p_\alpha x_2$. The matrix B_{ijk}^α is obtained from elastic constants C_{ijkl} by

$$B_{ijk}^\alpha = C_{ijk1} + p_\alpha C_{ijk2}.$$

The six roots p_α are the imaginary numbers, for which the following determinant is null

$$|\{B_{i1k}^\alpha + p_\alpha B_{i2k}^\alpha\}| = 0. \tag{2}$$

The vectors A_k^α, associated to each root p_α, are the non-null vectors that verify the relation

$$(B_{i1k}^\alpha + p_\alpha B_{i2k}^\alpha) A_k^\alpha = 0. \tag{3}$$

In all the above expressions and in the followings, we use the Einstein summation convention on repeated indexes, except for Greek indexes α that design the different roots p_α. Such summations on α will always be explicitly indicated as in Eq. (1).

The six roots p_α are necessary complex. If p_α is a solution of Eq. (2), then its complex conjugate $p_\alpha{}^*$ is also a solution. We sort the roots p_α according to the following usual rule

$$\Im(p_\alpha) > 0 \text{ and } p_{\alpha+3} = p_\alpha{}^*, \quad \forall\alpha \in [1:3], \tag{4}$$

where $\Im(p_\alpha)$ is the imaginary part of p_α. With such a convention, the matrices B_{ijk}^α verify the relation

$$B_{ijk}^{\alpha+3} = B_{ijk}^\alpha{}^*, \tag{5}$$

and the vectors A_k^α can be chosen so that

$$A_k^{\alpha+3} = A_k^{\alpha *}. \tag{6}$$

As the elastic displacement has to be real, the functions f_α have also the property

$$f_{\alpha+3}(z^*) = f_\alpha(z)^*. \tag{7}$$

The general form of the function f_α defining the elastic displacement and the stress (Eq. 1) is a Laurent series[15]. If we restrict ourselves to a line defect in an infinite crystal, the series is limited to the following terms

$$f_\alpha(z) = \mp\frac{1}{2\pi\mathrm{i}}\left(D_\alpha \ln(z) + \sum_{k=-\infty}^{1} C_\alpha^k z^k\right), \tag{8}$$

with $\mathrm{i} = \sqrt{-1}$. The sign $\mp$ in this equation has to be taken as $-$ for $1 \leq \alpha \leq 3$ (roots having a positive imaginary part) and $+$ for $4 \leq \alpha \leq 6$ (roots having a negative imaginary part). $\ln(z)$ is the principal determination of the complex logarithm, whose imaginary part belongs to $[-\pi : \pi[$, thus showing a discontinuity in $\mathbb{R}^-$.

Far from the line defect, the main contribution to the function f_α, and thus to the elastic displacement, arises from the logarithm term. This corresponds to the Volterra elastic field created by a dislocation and to the 2D elastic Green function for a line force. Close to the line defect, the other terms in Eq. (8) may also lead to a relevant contribution. For a dislocation, these additional terms describe the core field. In the following, we only consider the main contribution to the core field corresponding to the term $k = 1$ in the Laurent series. This correctly describes the core field far enough from the line defect. The superposition of the Volterra and of the core fields, which gives the total elastic field created by a line defect, is then obtained from the following truncated series

$$f_\alpha(z) \underset{r\to\infty}{\sim} \mp\frac{1}{2\pi\mathrm{i}}\left(D_\alpha \ln(z) + C_\alpha^{-1}\frac{1}{z}\right).$$

A. Volterra elastic field

The Volterra elastic field is given by the logarithm in Eq. (8). This leads to the following displacement and stress fields

$$u_k^{\mathrm{V}}(\mathbf{x}) = \frac{1}{2}\sum_{\alpha=1}^{6} \mp\frac{1}{2\pi\mathrm{i}} A_k^\alpha D_\alpha \ln(z_\alpha), \tag{9a}$$

$$\sigma_{ij}^{\mathrm{V}}(\mathbf{x}) = \frac{1}{2}\sum_{\alpha=1}^{6} \mp\frac{1}{2\pi\mathrm{i}} B_{ijk}^\alpha A_k^\alpha D_\alpha \frac{1}{z_\alpha}. \tag{9b}$$

This corresponds to the long range elastic field of a dislocation of Burgers vector $\mathbf{b}$ or a line force of amplitude $\mathbf{F}$ if the coefficients D_α verify the system of equations[15]

$$\frac{1}{2}\sum_{\alpha=1}^{6} A_k^\alpha D_\alpha = -b_k,$$
$$\frac{1}{2}\sum_{\alpha=1}^{6} B_{i2k}^\alpha A_k^\alpha D_\alpha = -F_i. \tag{10}$$

Stroh[16,17] proposed a simple solution to this system of equations. In that purpose, he defined a new vector

$$L_i^\alpha = B_{i2k}^\alpha A_k^\alpha = -\frac{1}{p_\alpha} B_{i1k}^\alpha A_k^\alpha. \tag{11}$$

As the vectors A_i^α are defined through the equation (3), their norm is not fixed. One can therefore choose their norm so that

$$2A_i^\alpha L_i^\alpha = 1, \quad \forall\alpha. \tag{12}$$

Stroh showed that such a definition of the vectors A_i^α and L_i^α leads to the orthogonality property

$$A_i^\alpha L_i^\beta + A_i^\beta L_i^\alpha = \delta_{\alpha\beta},$$

where $\delta_{\alpha\beta}$ is the Kronecker symbol. These vectors also verify the following relations[17,18]

$$\sum_{\alpha=1}^{6} A_i^\alpha A_j^\alpha = 0, \quad \sum_{\alpha=1}^{6} L_i^\alpha L_j^\alpha = 0 \quad \text{and} \quad \sum_{\alpha=1}^{6} A_i^\alpha L_j^\alpha = \delta_{ij}.$$

These orthogonality properties lead to the expression of the coefficient D_α:

$$D_\alpha = -2\left(L_i^\alpha b_i + A_i^\alpha F_i\right). \tag{13}$$

B. Core field

The Volterra solution models the elastic field created by a dislocation far enough from the dislocation core. Close to the core, the dislocation core field may be relevant too. We model this additional elastic field by considering the term $1/z$ in Eq. (8). Gehlen *et al.*[9] have shown that this term may be obtained from dipoles of line forces. It is also possible to consider dipoles of dislocations, which may be more natural to model the core field of a dissociated dislocation. Therefore, we assume that the core field can be modeled by an equilibrated distribution of dislocations and line forces of force amplitude $\mathbf{F}^q$ and of Burgers vector $\mathbf{b}^q$ located at $\mathbf{a}^q$. All line force and dislocation directions are assumed to be collinear to $\mathbf{e}_3$. As the distribution is equilibrated, the resultant of the forces and the total Burgers vector have to vanish

$$\sum_q \mathbf{F}^q = \mathbf{0} \quad \text{and} \quad \sum_q \mathbf{b}^q = \mathbf{0}. \tag{14}$$

The elastic displacement and the stress of this distribution is given by the superposition of the Volterra elastic field created by each line defect

$$u_k^{\mathrm{c}}(\mathbf{x}) = \sum_q u_k^{\mathrm{V}^{(q)}}(\mathbf{x} - \mathbf{a}^q),$$
$$\sigma_{ij}^{\mathrm{c}}(\mathbf{x}) = \sum_q \sigma_{ij}^{\mathrm{V}^{(q)}}(\mathbf{x} - \mathbf{a}^q).$$

We then assume that the norm of $\mathbf{x}$ is large compared to the norm of the vectors $\mathbf{a}^q$. One can thus make a limited expansion[9,11,18,19] leading to

$$u_k^{\mathrm{c}}(\mathbf{x}) = -\sum_q \frac{\partial u_k^{\mathrm{V}^{(q)}}(\mathbf{x})}{\partial x_m} a_m^q + O\left(\|\mathbf{a}^q\|^2\right),$$
$$\sigma_{ij}^{\mathrm{c}}(\mathbf{x}) = -\sum_q \frac{\partial \sigma_{ij}^{\mathrm{V}^{(q)}}(\mathbf{x})}{\partial x_m} a_m^q + O\left(\|\mathbf{a}^q\|^2\right),$$

where we have used Eq. (14) to eliminate the first term of the expansion. Using Eq. (9) and taking the limit $\mathbf{a}^q \to \mathbf{0}$, one finally obtains the expression of the core field

$$u_k^{\mathrm{c}}(\mathbf{x}) = \frac{1}{2}\sum_{\alpha=1}^{6} \mp\frac{1}{2\pi\mathrm{i}} A_k^\alpha C_\alpha^{-1} \frac{1}{x_1 + p_\alpha x_2}, \tag{15a}$$

$$\sigma_{ij}^{\mathrm{c}}(\mathbf{x}) = \frac{1}{2}\sum_{\alpha=1}^{6} \pm\frac{1}{2\pi\mathrm{i}} B_{ijk}^\alpha A_k^\alpha C_\alpha^{-1} \frac{1}{\left(x_1 + p_\alpha x_2\right)^2}, \tag{15b}$$

with

$$C_\alpha^{-1} = 2A_i^\alpha\left(M_{i1} + p_\alpha M_{i2}\right) + 2L_i^\alpha\left(P_{i1} + p_\alpha P_{i2}\right),$$

where M and P are respectively the first moment tensors of the line force and of the dislocation distribution

$$M_{ij} = \sum_q F_i^q a_j^q \quad \text{and} \quad P_{ij} = \sum_q b_i^q a_j^q.$$

As we assume that the distribution of line defects representative of the core field is equilibrated, it does not produce any torque. This implies that the tensor M_{ij} is symmetric[18]. The first moment tensors M and P can be simply deduced from the homogeneous stress computed in atomistic simulations using periodic boundary conditions[6]. Another method based on path-independent interaction integrals computed through the field observed in atomistic simulations has also been proposed[20,21].

III. ELASTIC ENERGY OF AN ISOLATED LINE DEFECT

We now calculate the elastic energy of a line defect, such as a dislocation, taking into account its core field. The elastic field created by the line defect is thus the superposition of the Volterra solution given by Eq. (9) and of the core field given by Eq. (15). We define the elastic energy of the line defect as the integral of the elastic energy density over the volume in-between two cylinders centered on the line defect. The inner cylinder of radius r_{c} isolates the line defect core: elastic fields are diverging at the line defect position and one needs to exclude the core region, where elasticity breaks down. The external cylinder of radius R_∞ is introduced to prevent the elastic energy from diverging. Then, Gauss theorem allows us to obtain the elastic energy

$$E = \frac{1}{2}\oint_S \left(\sigma_{ij}^{\mathrm{V}} + \sigma_{ij}^{\mathrm{c}}\right)\left(u_i^{\mathrm{V}} + u_i^{\mathrm{c}}\right) \mathrm{d}S_j, \tag{16}$$

where the integration surface S is composed of both cylinder surfaces and the branch cut, which isolates the displacement discontinuity. We consider cylinders of unit height so as to express the elastic energy per unit length of line defect.

This elastic energy can be decomposed into three different contributions: the contribution of the Volterra solution, the contribution of the core field and the cross interaction between both elastic fields.

A. Volterra contribution

The Volterra contribution corresponds to the product $\sigma_{ij}^{\mathrm{V}} u_i^{\mathrm{V}}$ in Eq. (16). It is given by the well-known result[16,17,22]

$$E^{\mathrm{V}} = \frac{1}{2}\left(b_i K_{ij}^0 b_j + F_i K_{ij}'^0 F_j\right) \ln\left(\frac{R_\infty}{r_{\mathrm{c}}}\right), \tag{17}$$

where we have defined the second rank tensors

$$K_{ij}^0 = \sum_{\alpha=1}^{6} \pm\frac{1}{2\pi \mathrm{i}} L_i^\alpha L_j^\alpha \text{ and } K_{ij}'^0 = \sum_{\alpha=1}^{6} \mp\frac{1}{2\pi \mathrm{i}} A_i^\alpha A_j^\alpha. \tag{18}$$

B. Core field contribution

The contribution of the core field to the elastic energy corresponds to the product $\sigma_{ij}^{\mathrm{c}} u_i^{\mathrm{c}}$ in Eq. (16). As the core field does not create any displacement discontinuity, the integration surface is simply composed of the inner and the external cylinders. This leads to the contribution

$$\begin{aligned} E^{\mathrm{c}} = -\frac{1}{8} \sum_{\alpha=1}^{6} \mp\frac{1}{2\pi\mathrm{i}} A_i^\alpha C_\alpha^{-1} \\ \sum_{\beta=1}^{6} \pm\frac{1}{2\pi\mathrm{i}} \left[B_{i1k}^\beta I_x^3(p_\alpha, p_\beta) + B_{i2k}^\beta I_y^3(p_\alpha, p_\beta)\right] \\ A_k^\beta C_\beta^{-1} \left(\frac{1}{{r_{\mathrm{c}}}^2} - \frac{1}{{R_\infty}^2}\right). \end{aligned}$$

The integrals $I_x^3(p,q)$ and $I_y^3(p,q)$ are defined in the Appendix (Eq. (A.1)). We use the fact that $I_x^3(p,q) = -p I_y^3(p,q)$ as well as the property verified by the vectors A_k^α (Eq. 3) and the definition of the vectors L_i^α (Eq. 11) to obtain

$$\begin{aligned} E^{\mathrm{c}} = -\frac{1}{32\pi^2} \sum_{\alpha=1}^{6} \pm \sum_{\beta=1}^{6} \pm C_\alpha^{-1} A_i^\alpha L_i^\beta C_\beta^{-1} \left[p_\alpha p_\beta + 1\right] \\ I_y^3(p_\alpha, p_\beta) \left(\frac{1}{{r_{\mathrm{c}}}^2} - \frac{1}{{R_\infty}^2}\right). \end{aligned}$$

Finally, the expression of the integral $I_y^3(p,q)$ given in the appendix allows us to write

$$\begin{aligned} E^{\mathrm{c}} = \frac{1}{4\pi} \Im\left(\sum_{\alpha=1}^{3}\sum_{\beta=1}^{3} \frac{1+p_\alpha {p_\beta}^*}{(p_\alpha - {p_\beta}^*)^2} C_\alpha^{-1} A_i^\alpha {L_i^\beta}^* {C_\beta^{-1}}^*\right) \\ \left(\frac{1}{{r_{\mathrm{c}}}^2} - \frac{1}{{R_\infty}^2}\right). \end{aligned} \tag{19}$$

The dependence of this expression with R_∞ shows that the elastic energy of the core field is concentrated close to the line defect. It is possible to take the limit $R_\infty \to \infty$, and thus to define an elastic energy associated with the core field in the whole volume excluding the core region, where elasticity breaks down.

C. Volterra - core field interaction

Then we calculate the interaction energy between both elastic fields created by the line defect. Two different integrals can be used to obtain this interaction energy[18]:

$$E^{\mathrm{V-c}} = \oint_S \sigma_{ij}^{\mathrm{V}} u_i^{\mathrm{c}} \mathrm{d}S_j = \oint_S \sigma_{ij}^{\mathrm{c}} u_i^{\mathrm{V}} \mathrm{d}S_j.$$

We rather use the first definition to evaluate $E^{\mathrm{V-c}}$: as the core field displacement $\mathbf{u}^{\mathrm{c}}$ does not show any discontinuity except at the origin, the integration surface of the first integral is simply composed of the inner and external cylinders. This leads to the following interaction energy

$$\begin{aligned} E^{\mathrm{V-c}} = \frac{1}{4} \sum_{\alpha=1}^{6} \mp\frac{1}{2\pi\mathrm{i}} A_i^\alpha C_\alpha^{-1} \\ \sum_{\beta=1}^{6} \mp\frac{1}{2\pi\mathrm{i}} \left(B_{i1k}^\beta I_x^2(p_\alpha, p_\beta) + B_{i2k}^\beta I_y^2(p_\alpha, p_\beta)\right) A_k^\beta D_\beta \\ \left(\frac{1}{r_{\mathrm{c}}} - \frac{1}{R_\infty}\right). \end{aligned}$$

The integrals $I_x^2(p,q)$ and $I_y^2(p,q)$ are defined in the appendix (Eq. (A.2)). As these integrals vanish for any values of p and q, this leads to $E^{\mathrm{V-c}} = 0$. As a result, there is no interaction energy between the Volterra elastic field and the core field of the line defect, and the elastic energy of a line defect is simply the sum of the elastic energies of the Volterra field and of the core field. Of course, this is true only when the Volterra and the core fields are centered at the same point. This may be imposed by symmetry, as for the $\langle 111 \rangle$ screw dislocation in a cubic crystal.[6,23] When the Volterra and the core fields have different centers,[4,5,9,12] an interaction energy between both elastic fields exists. Such a cross term can be simply calculated by considering the interaction of the core field with the stress created by the Volterra field, as described in the next section.

IV. INTERACTION WITH A STRESS FIELD

We now consider the interaction energy between an external stress field $\sigma_{ij}^{\mathrm{ext}}$ and a line defect. The external stress can be an applied stress or the stress originating from another defect. The line defect is located at the origin and its line direction is $\mathbf{e}_3$. It is characterized by its Burgers vector $\mathbf{b}$, its force resultant $\mathbf{F}$ and the first moments tensors M_{ij} and P_{ij}. The interaction energy can be decomposed into two contributions: the interaction with the Volterra elastic field and the interaction with the core field. The first contribution is well known.[1,18] For a dislocation, it is given by the integral of $\sigma_{ij}^{\mathrm{ext}} b_i \mathrm{d}S_j$ along the dislocation cut, where $\mathrm{d}S_j$ is an infinitesimal surface vector. For a line force, it is given by the scalar product $F_i u_i^{\mathrm{ext}}$, where u_i^{ext} is the displacement associated to the external stress field. We now determine the contribution of the core field to the interaction energy $E_{\rm c}^{\rm inter}$.

A. Core field contribution

The interaction energy of the core field with the stress field $\sigma_{ij}^{\rm ext}$ can be obtained by considering the line defect distribution responsible for the core field, thus using the same approach as used by Siems[18,24] for a point defect. The interaction energy is then given by

$$E_{\rm c}^{\rm inter} = \sum_q \int_0^1 \sigma_{ij}^{\rm ext}(\lambda \mathbf{a}^q) b_i^q \epsilon_{jk3} a_k^q {\rm d}\lambda - F_i^q u_i^{\rm ext}(\mathbf{a}^q),$$

where ϵ_{jkl} is the permutation tensor. The first term represents the interaction with the different dislocations of the distribution ($\epsilon_{jk3} a_k^q {\rm d}\lambda$ is the infinitesimal surface vector along the dislocation cut), and the second term represents the interaction with the line forces. A limited expansion of $\sigma_{ij}^{\rm ext}$ and of $u_i^{\rm ext}$ at the origin leads to

$$E_{\rm c}^{\rm inter} = \sum_q \sigma_{ij}^{\rm ext}(\mathbf{0}) b_i^q \epsilon_{jk3} a_k^q - F_i^q \frac{\partial u_i^{\rm ext}(\mathbf{0})}{\partial x_j} a_j^q + O\left(\|\mathbf{a}^q\|^2\right).$$

We finally use the fact that the tensor M_{ij} is symmetric and take the limit $\mathbf{a}^q \to \mathbf{0}$ to obtain the interaction energy

$$E_{\rm c}^{\rm inter} = \sigma_{ij}^{\rm ext}(\mathbf{0}) \left(\epsilon_{jk3} P_{ik} - S_{ijkl} M_{kl}\right), \qquad (20)$$

where the elastic compliances S_{ijkl} are the inverse of the elastic constants ($S_{ijkl} C_{klmn} = \frac{1}{2}\left(\delta_{im}\delta_{jn} + \delta_{in}\delta_{jm}\right)$).

Thus Eq. (20) shows that an additional contribution needs to be considered in the interaction energy of a line defect with a stress when a core field is present. In particular, this contribution of the core field leads to a dislocation-pressure interaction which can modify the kink formation energy and the dislocation line tension at high pressures[3]. Such a dependence of the dislocation energy with the pressure has been observed in atomistic simulations[25–27]. Eq. (20) should allow to model this dependence, or at least the first order variation.

B. Force acting on a line defect

The external stress field $\sigma_{ij}^{\rm ext}$ creates on the line defect a force which derives from the interaction energy. Without the core field, this force would be simply given by the Peach-Koehler formula for a pure dislocation and by the product $-S_{ijkl}\sigma_{kl}^{\rm ext} F_j$ for a pure line force. Because of the core field, there is an additional force $\mathbf{f}^{\rm c}$ acting on the line defect. This force derives from the interaction energy given by Eq. (20)

$$f_n^{\rm c} = -\frac{\partial \sigma_{ij}^{\rm ext}(\mathbf{0})}{\partial x_n}\left(\epsilon_{jk3} P_{ik} - S_{ijkl} M_{kl}\right). \qquad (21)$$

Because of the core field, there is a force acting on the line defect, which is proportional to the gradient of the applied stress.

C. Elastic energy of an isolated dipole

The calculation of the elastic energy of an isolated dislocation dipole is one important application, where one needs to calculate the interaction energy of a line defect with a stress field. In that case, the external stress field is created by the other line defect composing the dipole. Here we determine the elastic energy of a dislocation dipole that is assumed to be isolated from any other defect. This elastic energy is defined as the integral of the energy density on the whole volume except two cylinders of radius $r_{\rm c}$ excluding the regions around the dislocation core. As the elastic energy is now converging, we do not need to introduce an external cylinder as we did for an isolated dislocation. The dipole is composed of two line defects of opposite Burgers vector $\mathbf{b}$ and opposite force resultant $\mathbf{F}$ having the same core field characterized by the moment tensors M_{ij} and P_{ij}. We assume that $\mathbf{e}_3$ corresponds to the line direction of the dislocations. The dipole is then defined by the distance d between the two dislocations and by the angle ϕ between the dipole direction and a reference vector $\mathbf{e}_1$.

If the elastic field created by each dislocation composing the dipole is only of the Volterra type [Eq. (9)], the elastic energy of the dipole is

$$E_{\rm dipole}^{\rm V} = \left(b_i K_{ij}^0 b_j + F_i K_{ij}^{\prime 0} F_j\right) \ln\left(\frac{d}{r_{\rm c}}\right) + 2E_{\rm c}^{\rm V}(\phi), \qquad (22)$$

where the tensors K_{ij}^0 and $K_{ij}^{\prime 0}$ are given by Eq. (18). $E_{\rm c}^{\rm V}$ is the contribution from core tractions to the elastic energy. Such a contribution arises from the work done by the tractions of the Volterra elastic field exerted on the cylinders that isolate the dislocation cores. It exists even when the core field is neglected and it is given by[28]

$$E_{\mathrm{c}}^{\mathrm{V}}(\phi) = \frac{1}{8}\sum_{\alpha=1}^{6}\ln\left(\mathrm{i}\pm p_\alpha\right)\sum_{\beta=1}^{6}\pm\frac{1}{2\pi\mathrm{i}}D_\alpha\left(A_i^\alpha L_i^\beta - L_i^\alpha A_i^\beta\right)D_\beta + \frac{1}{8\pi\mathrm{i}}\sum_{\alpha=1}^{3}\sum_{\beta=4}^{6}D_\alpha\left(A_i^\alpha L_i^\beta - L_i^\alpha A_i^\beta\right)D_\beta\ln\left(p_\alpha - p_\beta\right)$$
$$+\frac{1}{2}\sum_{\alpha=1}^{6}\pm\frac{1}{2\pi\mathrm{i}}\left(b_i L_i^\alpha L_j^\alpha b_j - F_i A_i^\alpha A_j^\alpha F_j\right)\ln\left(\cos\phi + p_\alpha\sin\phi\right).$$

Considering now that a core field as described by Eq. (15) is also created by each dislocation, one has to add to the elastic energy of the dipole [Eq. (22)] the contribution from the core field of each dislocation, $2E^{\mathrm{c}}$, as given by Eq. (19) in the limit $R_\infty \to \infty$.

Another contribution also needs to be taken into account in the elastic energy when dislocations create both a Volterra and a core field. It arises from the interaction of the total stress field created by the first dislocation with the core field of the second one, and vice versa. This interaction energy can be calculated using Eq. (20), which leads to the result

$$E_{\mathrm{dipole}}^{\mathrm{V-c}} = \left(2\sigma_{ij}^{\mathrm{V}}(\mathbf{d}) + \sigma_{ij}^{\mathrm{c}}(\mathbf{d})\right)\left(\epsilon_{jk3}P_{ik} - S_{ijkl}M_{kl}\right), \quad (23)$$

where the vector $\mathbf{d}$ is defined by the coordinates $d(\cos\phi, \sin\phi, 0)$. Equation (23) shows that the elastic energy of the dipole now contains a contribution varying with the inverse of the distance d and another contribution varying with the square of the inverse of d.

D. Dislocation dipole in periodic boundary conditions

When studying dislocations in atomistic simulations, one can use periodic boundary conditions. A dipole is introduced to ensure that the total Burgers vector of the simulation box is null. Atomic simulations allow obtaining the excess energy associated with the defects present in the simulation box. One can deduce from this quantity dislocation intrinsic energy properties such as their core energy. To do so, one needs to calculate the elastic energy contained in the simulation box. This elastic energy includes the elastic energy of the primary dipole as well as half the interaction energy with all its periodic images. When the simulation box is small, as in *ab initio* calculations, one needs to consider not only the Volterra field but also the core field of the dislocations when computing the elastic energy[6].

The elastic energy of the primary dipole is given in the preceding section. The interaction energy between two dipoles can be obtained by decomposing it into the contributions arising from the different constituents of the elastic field. The interaction energy arising from the Volterra field of each dipole is obtained thanks to the expression given by Stroh[16] for the interaction energy between two dislocations. If the coordinates of the vectors joining the two dislocations are (x_1, x_2, x_3), this part of the interaction energy is given by

$$E_{\mathrm{inter}}^{\mathrm{V-V}} = -\sum_{\alpha=1}^{6}\pm\frac{1}{2\pi\mathrm{i}}b_i^{(1)}L_i^\alpha L_j^\alpha b_j^{(2)}\ln\left(x_1 + p_\alpha x_2\right),$$

where $\mathbf{b}^{(1)}$ and $\mathbf{b}^{(2)}$ are the respective Burgers vectors of each dislocation[29].

The part of the interaction energy arising from the core field is obtained thanks to Eq. (20). The external stress $\sigma_{ij}^{\mathrm{ext}}$ appearing in this equation corresponds to the stress created by the other dislocations, where both the Volterra and the core fields are considered.

When summing all contributions from the different periodic images, one should be aware that the sums are only conditionally convergent. This convergence problem can be easily resolved using the regularization method of Cai *et al.*[30].

V. CONCLUSIONS

We have extended in this paper the approach of Hirth and Lothe[11] to model dislocation core fields within linear anisotropic elasticity theory by deriving the elastic energy of a straight dislocation while taking full account of its core field. The obtained expression shows that this elastic energy is the sum of the energies corresponding to the Volterra field and to the core field, and that no cross interaction exists between these two elastic fields. We have also shown that the core field leads to an additional contribution to the interaction energy between a dislocation and an external stress. Through this contribution, the energy of a dislocation can depend on the applied pressure. This interaction with the core field is also responsible for an additional force acting on the dislocation, which is proportional to the gradient of the applied stress. Dislocation properties may therefore be affected in regions where a high-stress gradient is present such as in a dislocation pile-up[7,8] or close to a crack tip.

The interaction of the dislocations caused by their core field is shorter-range than their interaction through their Volterra field. It will therefore affect the interaction between dislocations when they get close enough. Such a situation may arise in atomistic simulations, where the size of the simulation box may be too small to neglect the influence of the core field.[6] One should then take account of the dislocation core field when calculating elastic energies, which can be done using the different expressions of this paper. An example is given in the following paper,[23] where the developed formalism is applied to the $\langle 111 \rangle$ screw dislocation in α-iron.

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Appendix: Integrals

The elastic energy of the core field (*cf.* §III B) makes the two following integrals appear

$$I_x^3(p,q) = \int_{-\pi}^{\pi} \frac{\cos\theta}{(\cos\theta + p\sin\theta)(\cos\theta + q\sin\theta)^2} \mathrm{d}\theta,$$
$$I_y^3(p,q) = \int_{-\pi}^{\pi} \frac{\sin\theta}{(\cos\theta + p\sin\theta)(\cos\theta + q\sin\theta)^2} \mathrm{d}\theta. \tag{A.1}$$

These integrals of a rational function of $\cos(\theta)$ and $\sin(\theta)$ can be evaluated using the residues theorem[31]. This leads to the result

$$\begin{aligned} I_x^3(p,q) &= 0 & &\text{if } \Im(p) > 0 \text{ and } \Im(q) > 0, \\ &= \frac{4\pi \mathrm{i} p}{(p-q)^2} & &\text{if } \Im(p) > 0 \text{ and } \Im(q) < 0, \\ &= \frac{-4\pi \mathrm{i} p}{(p-q)^2} & &\text{if } \Im(p) < 0 \text{ and } \Im(q) > 0, \\ &= 0 & &\text{if } \Im(p) < 0 \text{ and } \Im(q) < 0, \end{aligned}$$

$$\begin{aligned} I_y^3(p,q) &= 0 & &\text{if } \Im(p) > 0 \text{ and } \Im(q) > 0, \\ &= \frac{-4\pi \mathrm{i}}{(p-q)^2} & &\text{if } \Im(p) > 0 \text{ and } \Im(q) < 0, \\ &= \frac{4\pi \mathrm{i}}{(p-q)^2} & &\text{if } \Im(p) < 0 \text{ and } \Im(q) > 0, \\ &= 0 & &\text{if } \Im(p) < 0 \text{ and } \Im(q) < 0. \end{aligned}$$

The two integrals appearing in the interaction energy between the Volterra and the core fields of a line defect (*cf.* §III C) are

$$I_x^2(p,q) = \int_{-\pi}^{\pi} \frac{\cos\theta}{(\cos\theta + p\sin\theta)(\cos\theta + q\sin\theta)} \mathrm{d}\theta$$
$$I_y^2(p,q) = \int_{-\pi}^{\pi} \frac{\sin\theta}{(\cos\theta + p\sin\theta)(\cos\theta + q\sin\theta)} \mathrm{d}\theta \tag{A.2}$$

The residues theorem leads to the result $I_x^2(p,q) = I_y^2(p,q) = 0$.

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